

Analyzing Single Crystal Time-of-Flight Neutron Data - NOBUGS2002/030

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Software for time-of-flight single crystal diffractometer (SCD) data visualization and analysis was originally written to be run in batch mode on VMS-VAX systems. Modern computers and software tools allow a new level of visualization and user interaction. The Integrated Spectral Analysis Workbench (ISAW) is being extended and customized for SCD measurements. To this end, new viewers and operators have been added to ISAW. One of the new operators allows running a program written in another language, such as C or FORTRAN, to integrate tested software into the object-oriented package. This provides a method for preserving earlier software development while making use of modern tools.

I. INTRODUCTION

The single crystal diffractometer (SCD) at the intense pulsed neutron source (IPNS) was the among first of its kind when it was built. It uses a four circle Huber diffractometer with the chi angle fixed at 45 degrees and a single anger camera at 90 degrees from the direct beam at ~ 30 cm from the sample. The detector has 85×85 pixels in an active area of $30 \text{ cm} \times 30 \text{ cm}$.¹ This has been the instrument configuration, with minor adjustments, ever since. SCD is currently going through a major upgrade, replacing its original detector with two higher resolution anger cameras that each have an active area of $15 \text{ cm} \times 15 \text{ cm}$ at a distance of ~ 20 cm from the sample. In addition, the data acquisition system (DAS) for the SCD is also being upgraded. Not surprisingly the entire instrument upgrade is making it necessary to update much of the analysis software.

The Integrated Spectral Analysis Workbench (ISAW) is a general purpose data analysis and visualization package which can read the raw data of any IPNS instrument, including the upgraded SCD. ISAW also has an extendible system for performing calculations and operations on the data well suited to developing new analysis methods. This paper will describe the new data analysis package. Its early versions use much of the old software while implementing new methods of data visualization.

II. CURRENT SOFTWARE

The intention of all measurements on SCD is to collect up to 2π steradians of diffraction data from a single crystal sample. The raw data is then reduced to Bragg intensities consisting of the (hkl) index, integrated intensity, and uncertainty in the integrated intensity. This information is then used to determine the contents of the unit cell. To measure the full 2π steradians up to 44 crystal orientations need to be measured. For many crystals this is unnecessary and far fewer orientations are measured to reveal all of the unique reflections. An example of this

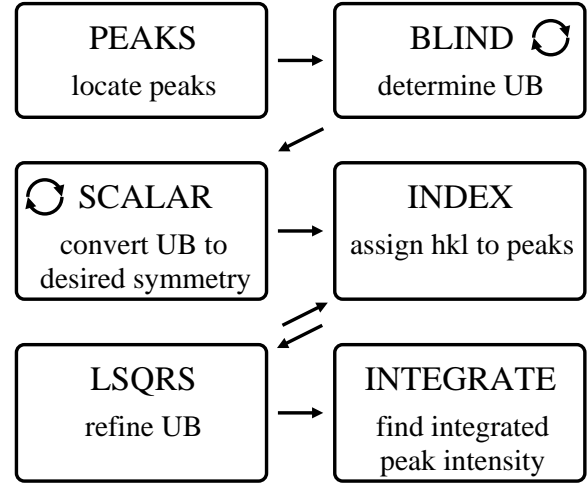


FIG. 1: Outline of the data analysis to produce a list of indexed, integrated peak intensities.

is quartz, with a hexagonal crystal structure, which only needs 13 crystal orientations measured to collect all of the unique reflections.

The original analysis software was written using FORTRAN77 to run in a batch mode on the VAX. The analysis steps are outlined in Fig. 1. After the analysis is completed the list of reflections, frequently called peaks, are then converted to a format appropriate for the modeling software used. PEAKS determines the location of the brightest points in time and pixel space which is converted to position and wavelength. This is normally run once for each crystal orientation and all reflections are collected in the same file. Then BLIND is run repetitively with between 10 and 17 reflections to determine lattice parameters $(a, b, c, \alpha, \beta, \gamma)$ and an orientation matrix (UB) which are satisfactory.^{2,3} SCALAR transforms the symmetry of the UB matrix found with BLIND to be more appropriate. For the quartz example mentioned above the UB matrix determined by BLIND will frequently make b the long axis, SCALAR performs

the rotation to make c the long axis consistent with convention. INDEX takes the orientation matrix from SCALAR and determines as many of the (hkl) indexes as possible. Then LSQRS uses the indexed peaks to refine the lattice parameters and the UB matrix, which is then used to run INDEX again to get (hkl) for more peaks. After a few iterations of INDEX and LSQRS almost all peaks are indexed and the lattice parameters and UB matrix are well established. The lattice parameters and UB matrix are then used one more time to INTEGRATE all possible reflection locations in the data and write a new peaks file with the integrated intensity.

III. NEW ANALYSIS PACKAGE

With the upgraded instrument comes two main concerns: the file format is being changed and most of the algorithms assume that there is only one detector. The first problem is dealt with by using ISAW which can already read the files from the new DAS. The first and last steps in the analysis, PEAKS and INTEGRATE respectively, are the only times that access to the raw data is necessary. For this reason they are the only ones that need to be modified to deal with the changing file format. This is accomplished by porting the FORTRAN code to Java. The other steps in the analysis can be wrapped so ISAW can have a straightforward method of stepping through the analysis. Wrapping the software allows for rapid development of the new analysis package and providing more time for dealing with the more difficult problem of a second detector. The process of wrapping and testing software is made significantly simpler through ISAW's operator mechanism. An operator is similar to a subroutine in most programming languages. Each operator is intended to be a single step in the analysis which can be executed in an orderly fashion. For this reason each of the steps outlined in the previous section becomes an operator. Then the operators can be linked together with a script in a very straightforward manner. At the time of publication the migration to ISAW has been completed through LSQRS, and porting INTEGRATE is expected to happen early in 2003.

IV. NEW METHODS OF DATA VISUALIZATION

Another feature of ISAW is a set of interactive and highly correlated viewers. Since the time when the original data visualization software was written for SCD there has been many improvements in computing. For this reason the new visualization software can show the data in ways that were previously not possible. In Fig. 2 a traditional raster plot created by ISAW is shown. To the right of the plot is a set of readouts that give information about the pixel being pointed at with the mouse. Included in this is the momentum transfer, \vec{Q} , and the

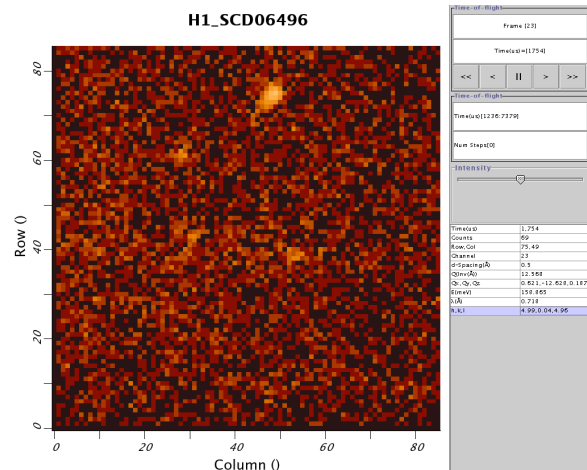


FIG. 2: The contour view in ISAW after the orientation matrix, UB , has been loaded. The selected intensity is the (550) peak of the data. The indexes are switched because the refined lattice has b as the long axes, contrary to convention.

index, (hkl) , which are both calculated while the user is interactively exploring the data. Future viewers planned include:

- Terrain view which is similar to the raster plot, but with the intensities plotted as height as well as color.
- Volume render which produces an overview of the full 3D data by accumulating and attenuating intensity values along rays through the data.
- Slicer that displays a set of three orthogonal intersecting planes that cut through the data. For example, three planes (h_0, k, l) , (h, k_0, l) , and (h, k, l_0) where the values of h_0 , k_0 , and l_0 are controlled interactively by the user.

Another view in its early development is a splatter plot which collects all points in \vec{Q} -space with an intensity above a threshold then plots them. This 3D view can be provides zooming and rotations to better explore the symmetry of the reflections.

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This figure "contour.jpg" is available in "jpg" format from:

<http://arXiv.org/ps/cond-mat/0210427v1>